Atomistic Simulations of Shock Waves in Polycrystalline Iron

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The propagation of shock waves through a polycrystalline iron sample is explored by large-scale atomistic simulations [1,2]. For large enough shock strengths the passage of the wave causes the body-centered-cubic (bcc) structure to transform into a close-packed structure with most structure being isotropic hexagonal-close-packed (hcp) and, depending on shock strength and grain orientation, some fraction of face-centered-cubic (fcc) structure [3]. The simulated shock state as represented by the Hugoniot is compared to experimental data (see Fig. 1). By calculating the extended x-ray absorption fine structure (EXAFS) directly from the atomic configurations obtained by our simulations [4], a comparison to recent experimental EXAFS measurements of nanosecond-laser shocks in polycrystalline iron shows that the experimental data are consistent with a phase transformation. However, the atomistically simulated EXAFS spectra also show that an experimental distinction between a product hcp or fcc phase is not possible based on the EXAFS spectra alone.

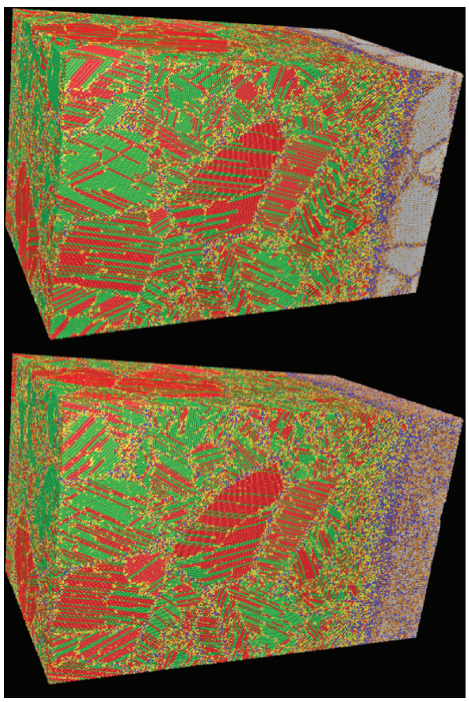

Fig. 1.
Experimental and simulated Hugoniots for polycrystalline iron. The full line is a linear fit to the experimental data [LANL data by Brown and McQueen], the dashed lines are fits to the three different parts of the simulated Hugoniots: elastic precursor, transformation wave, and the overdriven part. As a reference, the $[001]_{bcc}$ single crystalline shock data are included.

Figure 2 shows samples shocked with $u_p = 0.906$ km/s, 14.6 ps after the impact. Top (bottom) sample has an initial temperature of 50K (300K) and reaches a temperature behind the shock front of 296K (622K), pressures of about 39 GPa, and volume compressions of 19%. The samples consist of 32 grains and about 30 M atoms confined in a 57.4 nm x 7.4 nm x 109.9 nm box. Color coding denotes the local neighborhood of each atom: gray: bcc; blue: uniaxially compressed bcc; yellow: grain-boundary; red: hcp; and green: fcc. Fluctuations in the bcc structure at 300 K (bottom) wash out the color-scheme analysis, and therefore make it hard to see the grain boundary structure between the bcc grains. The hcp/fcc ratio behind the shock front is on average 1.5 for this shock strength and increases with decreasing shock strength. The initial average grain size—as defined by the average caliper diameter—is 32.7 nm.

The present simulations of shock waves in polycrystalline iron demonstrate how atomistic modeling can enhance our understanding of ultrafast dynamical processes that take place in shock-induced phase transformations. Interpretations of experimental data can be scrutinized and checked with the simulation data set (see Fig. 3).

Specifically, atomistically simulated and experimental EXAFS spectra both support the conclusion that a phase transformation polycrystalline iron takes place under shock loading, yielding an almost isotropic close-packed product phase. However, the simulations also reveal the possibility of the product having some sizable fraction of metastable fcc product, as opposed to purely

hcp. This question cannot be resolved from the experimental EXAFS spectra alone, since the noise-levels for those ultrafast in-situ measurements are too large to differentiate between hcp and fcc. We have to emphasize that details of the interatomic potential change the hcp to fcc ratio in the simulations. However, all tested EAM potentials for iron show a sizable fraction of fcc in the product phase under shock loading. Since the hcp/fcc ratio within a grain decreases the more the shock direction deviates from the $[001]_{bcc}$ direction with respect to the initial polycrystal, we speculate that there is a geometric component to this effect. The ABC stacking sequence along $[111]_{bcc}$ makes it easier to transform under rapid compression in this direction into the ABC-stacked fcc structure instead of the AB-stacked hcp phase. For shocks along $[001]_{bcc}$ the AB-stacked close-packed bcc planes transforming into the AB-stacked close-packed hcp planes more easily than into the ABC-stacked fcc planes. Fully resolved *ab-initio* molecular dynamics (MD) simulations would allow for a more reliable predication of the hcp to fcc ratio of the product phase. However, such methods are presently far too computationally intensive for the large scales needed for a polycrystalline system. Our nonequilibrium MD simulations were on the order of some 10 ps, still too short to detect further relaxation processes that might occur on longer time scales. We leave the final clarification of the detailed structure and relaxation of the product phase to planned high-energy laser-based experiments that can access time scales on the order of nanoseconds.

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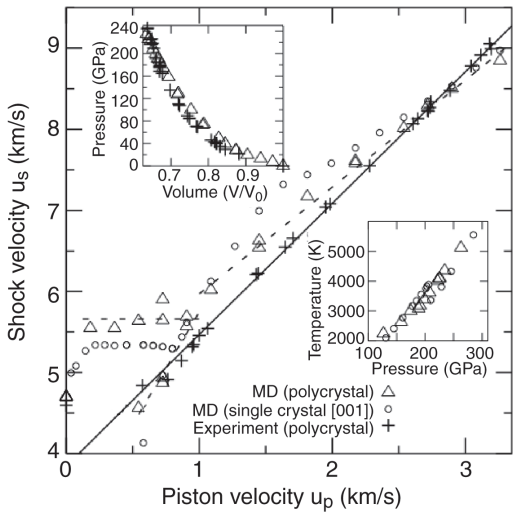

Fig. 2.
Samples shocked with u_p = 0.906 km/s, 14.6 ps after the impact. Please see the text for more details.

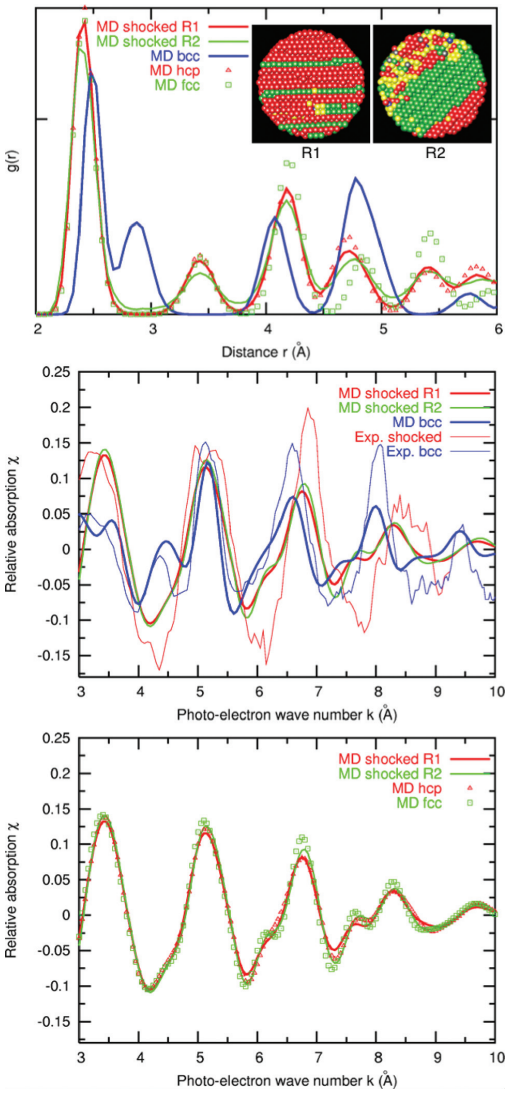

Fig. 3.
Radial distribution functions and EXAFS signal of several different cutouts (each containing about 5000 atoms) from the sample shown in Fig. 2 (bottom): purely bcc, region R1 (hcp/fcc ratio 3.2) and R2 (hcp/fcc ratio 1.03). The radial distribution and the EXAFS signals of the regions R1 and R2 are compared to ideal hcp and fcc structures simulated under the same pressure and temperature conditions. A comparison to experimental in situ EXAFS data are shown in the middle panel.